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An approximate approach to E-optimal designs for weighted polynomial regression by using Tchebycheff systems and orthogonal polynomials

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1 Introduction

In experimental designs, E-optimal designs are defined as designs which minimize the maximum eigenvalue of the covariance matrix of the estimator. The Tchebycheff systems sometimes play an important role in optimal designs.

We firstly give a brief introduction to E-optimal designs and Tchebycheff systems as preliminaries. Then an approximate approach to E-optimal designs for weighted polynomial regression is proposed.

2 E-optimal designs for linear regression and Tchebycheff systems

2.1 Linear regression and its E-optimal designs

A weighted linear regression model is defined by

$$Y = \theta^T f(x) + \varepsilon(x)$$

$$= \begin{pmatrix} \theta_0 & \theta_1 & \cdots & \theta_{m-1} \end{pmatrix} \begin{pmatrix} f_0(x) \\ f_1(x) \\ \vdots \\ f_{m-1}(x) \end{pmatrix} + \varepsilon(x),$$

where $f(x) = (f_0(x), f_1(x), \dots, f_{m-1}(x))^T$ is a vector of known linearly independent continuous functions, $\theta = (\theta_0, \theta_1, \dots, \theta_{m-1})$ is a vector of unknown parameters, and $\varepsilon(x)$ denotes a random error term. We call the functions $f_0(x), f_1(x), \dots, f_{m-1}(x)$ basis functions. Here we assume that the error term satisfies

$$E[\varepsilon(x)] = 0, \quad V[\varepsilon(x)] = \frac{\sigma^2}{w(x)},$$

where σ^2 is a positive constant and $w(x) \geq 0$ is called a weight function of regression.

Consider making N observations at experimental conditions $x_1, x_2, \dots, x_N \in \mathcal{X}$ such as

$$y_i = \theta^T f(x_i) + \varepsilon_i, \quad i = 1, 2, \dots, N$$

to estimate all unknown parameters $\theta_0, \theta_1, \dots, \theta_{m-1}$. Here the design space \mathcal{X} denotes the set of all possible points where observations can be made. Throughout this paper, we assume that different errors are uncorrelated, namely,

$$\mathbb{E}[\varepsilon_i] = 0, \quad \mathbb{V}[\varepsilon_i] = \frac{\sigma^2}{w(x_i)}, \quad \mathbb{E}[x_i x_j] = 0, \quad i, j = 1, 2, \dots, N, \quad i \neq j$$

even if they has the same experimental conditions $x_i = x_j$. From Gauss–Markov’s theorem, the best linear unbiased estimator $\hat{\theta}$ of the parameter vector θ is

$$\hat{\theta} = (X^T W X)^{-1} X^T W y, \quad (1)$$

where

$$\begin{aligned} X &= (f(x_1), f(x_2), \dots, f(x_N))^T \in M_{N,m}(\mathbb{R}), \\ W &= \text{diag}(w(x_1), w(x_2), \dots, w(x_N)) \in M_N(\mathbb{R}), \\ y &= (y_1, y_2, \dots, y_N)^T. \end{aligned}$$

It is well known that the its covariance matrix is

$$\text{Cov}[\hat{\theta}] = \sigma^2 (X^T W X)^{-1}. \quad (2)$$

Note that the weighted least squares estimator of the parameter vector θ is also given by (1).

The multiset $\{x_1, x_2, \dots, x_N\}$ of the experimental conditions is called a design, and it is considered as a probability measure μ such that

$$\mu(\{x\}) = \frac{\#\{i \mid x_i = x, \quad i = 1, 2, \dots, N\}}{N}.$$

Hereinafter we consider designs as probability measures. Since accuracy of estimators depend designs, it is important to choose a good design. There are various criteria for good designs, and some of them minimize the covariance matrix of estimators in some sense. In this paper, we consider E-optimal designs which minimize the maximum eigenvalue of the covariance matrix. Using the Fisher information matrix

$$\begin{aligned} M_{f,w}(\mu) &= \int_{\mathcal{X}} w(x) f(x) f(x)^T d\mu(x) \\ &= \int_{\mathcal{X}} \left(\sqrt{w(x)} f(x) \right) \left(\sqrt{w(x)} f(x) \right)^T d\mu(x), \end{aligned}$$

the covariance matrix (2) is rephrased as

$$\text{Cov}[\hat{\theta}] = \frac{\sigma^2}{N} M_{f,w}(\mu)^{-1}.$$

Hence E-optimal designs are defined as the probability measures which maximize the minimum eigenvalue of the Fisher information matrix. Namely, E-optimal designs are defined as the optimal solutions of the optimization problem

$$\text{maximize } \lambda_{\min}(M_{f,w}(\mu)) \quad \text{subject to } \mu \in \mathcal{P}_{\mathcal{X}} \quad (3)$$

where $\lambda_{\min}(A)$ denotes the minimum eigenvalue of the matrix A , and $\mathcal{P}_{\mathcal{X}}$ denotes the set of all probability measures on the Borel sets of \mathcal{X} . If the sample size N is fixed, all probabilities corresponding to the design μ must be multiple of $1/N$, however we do not consider this constraint. In this case, E-optimal designs are sometimes called approximate E-optimal designs instead of exact E-optimal designs. Thus, in this paper, we consider approximate E-optimal designs defined by (3), whose probabilities may be rounded to be multiples of $1/N$ in order to consider the corresponding multiset $\{x_1, x_2, \dots, x_N\}$. Then E-optimal designs no longer depend on the sample size N , they depend only the vector of functions

$$\begin{aligned} g(x) &= \begin{pmatrix} g_0(x) & g_1(x) & \cdots & g_{m-1}(x) \end{pmatrix}^T \\ &= \begin{pmatrix} \sqrt{w(x)}f_0(x) & \sqrt{w(x)}f_1(x) & \cdots & \sqrt{w(x)}f_{m-1}(x) \end{pmatrix}^T. \end{aligned} \quad (4)$$

For convenience, if the design μ is a discrete probability measure, then we write

$$\mu = \begin{pmatrix} s_1 & s_2 & \cdots & s_n \\ \rho_1 & \rho_2 & \cdots & \rho_n \end{pmatrix},$$

where s_1, s_2, \dots, s_n denote the support points of μ , and $\rho_k = \mu(\{s_k\})$, $k = 1, 2, \dots, n$.

See [3, 6] for details of optimal designs and other optimality criteria.

2.2 Tchebycheff systems and their applications to E-optimal designs

Let $u_1, u_2, \dots, u_n : I \rightarrow \mathbb{R}$ denote linearly independent continuous functions defined on a closed finite interval $I = [a, b]$. If there exists $\delta \in \{1, -1\}$ such that

$$\begin{aligned} a \leq t_1 < t_2 < \cdots < t_n \leq b \\ \Rightarrow \delta \det \left(u_i(t_j) \right)_{i,j=1}^n &= \delta \det \begin{pmatrix} u_1(t_1) & u_1(t_2) & \cdots & u_1(t_n) \\ u_2(t_1) & u_2(t_2) & \cdots & u_2(t_n) \\ \vdots & \vdots & \ddots & \vdots \\ u_n(t_1) & u_n(t_2) & \cdots & u_n(t_n) \end{pmatrix} > 0, \end{aligned}$$

then the set $\{u_1, u_2, \dots, u_n\}$ of functions is called a Tchebycheff system on I . Similarly, if there exists $\delta \in \{1, -1\}$ such that

$$a \leq t_1 < t_2 < \dots < t_n \leq b \Rightarrow \delta \det \left(u_i(t_j) \right)_{i,j=1}^n \geq 0,$$

then the set $\{u_1, u_2, \dots, u_n\}$ of functions is called a weak Tchebycheff system on I . It is well known [4, Theorem II 10.2] that the set $\{u_1, u_2, \dots, u_n\}$ is a weak Tchebycheff system if and only if there exists a unique function $\kappa(t)$ given by

$$\begin{aligned} \kappa(t) &= \gamma^T u(t), \\ \gamma &= \begin{pmatrix} \gamma_1 & \gamma_2 & \dots & \gamma_n \end{pmatrix}^T \in \mathbb{R}^n, \quad u(t) = \begin{pmatrix} u_1(t) & u_2(t) & \dots & u_n(t) \end{pmatrix}^T \end{aligned}$$

which satisfies the following two properties:

- (a) $|\kappa(t)| \geq C$ for all $t \in I$,
- (b) There exist n points s_1, s_2, \dots, s_n such that $a \leq s_1 < s_2 < \dots < s_n \leq b$ and $\kappa(s_k) = (-1)^k C$, $k = 1, 2, \dots, n$.

Here C is a fixed positive constant, usually which is set as 1. In this paper, we call the function $\kappa(t)$ a Tchebycheff function, and we call the points s_1, s_2, \dots, s_n Tchebycheff points.

If the set $\{g_0(x), g_1(x), \dots, g_{m-1}(x)\}$ is a weak Tchebycheff system on \mathcal{X} , then we can construct a design, called a Tchebycheff design, by the following procedure. Here $g_k(x) = \sqrt{w(x)} f_k(x)$, where $w(x)$ denotes a weight function of regression, $f_k(x)$ denotes a basis function. Let the Tchebycheff function $\kappa(x)$ be

$$\kappa(x) = \gamma^T g(x), \quad \gamma \in \mathbb{R}^m,$$

and let the Tchebycheff points of the Tchebycheff function $\kappa(x)$ be $s_1, s_2, \dots, s_m \in \mathcal{X}$. Then the Tchebycheff design μ^* is defined by

$$\begin{aligned} \mu^* &= \begin{pmatrix} s_1 & s_2 & \dots & s_m \\ \rho_1 & \rho_2 & \dots & \rho_m \end{pmatrix}, \\ \begin{pmatrix} \rho_1 & \rho_2 & \dots & \rho_m \end{pmatrix}^T &= \frac{F^{-1}\gamma}{\gamma^T \gamma}, \quad F = \left((-1)^{j+1} f_{i-1}(s_j) \right)_{i,j=1}^m. \end{aligned} \quad (5)$$

If the linear regression with the basis functions $f_0(x), f_1(x), \dots, f_{m-1}(x)$ has a unique E-optimal design, then the Tchebycheff design is the E-optimal design [5, pp. 94–97].

See [4] for more details of Tchebycheff systems.

3 An approximate approach to E-optimal designs for weighted polynomial regression

3.1 The proposed algorithm

Consider weighted polynomial regression, that is, consider the case of $f(x) = (1, x, \dots, x^{m-1})^T$. Thus $g(x)$ defined by (4) is $g(x) = \sqrt{w(x)}(1, x, \dots, x^{m-1})$ here. In this section, we propose an approximate approach to E-optimal designs for polynomial regression with almost general weight function.

At first we introduce to the E-optimal designs calculated exactly. The following theorem is shown by Dette [2].

Theorem 3.1. *Let the design space be $\mathcal{X} = [-1, 1]$, and let the weight function of regression be*

$$w(x) = (1-x)^\alpha(1+x)^\beta, \quad \alpha, \beta \in \{0, 1\}. \quad (6)$$

Then the set $\{g_0(x), g_1(x), \dots, g_{m-1}(x)\}$ is a weak Tchebycheff system, and the function

$$(1-x)^{\alpha/2}(1+x)^{\beta/2} J_{m-1}^{\alpha-1/2, \beta-1/2}(x) \quad (7)$$

is the Tchebycheff function. Here $J_n^{a,b}(x)$ denotes a Jacobi orthogonal polynomial

$$\begin{aligned} J_n^{(a,b)}(x) &= \frac{(-1)^n}{2^n n! (1-x)^a (1+x)^b} \frac{d^n}{dx^n} ((1-x)^{n+a} (1+x)^{n+b}) \\ &= \frac{1}{2^n} \sum_{k=0}^n \binom{n+a}{n-k} \binom{n+b}{k} (x-1)^k (x+1)^k. \end{aligned}$$

And the Tchebycheff function, calculated by (5), is the E-optimal design for polynomial regression with weight function (6).

We generalize this theorem by focusing that the Jacobi polynomial $J_n^{a,b}(x)$ is the orthogonal polynomial with respect to the weight function $\eta(x) = (1-x)^a(1+x)^b$, namely,

$$\int_{-1}^1 J_m^{(a,b)}(x) J_n^{(a,b)}(x) \eta(x) dx = \frac{2^{a+b+1} \Gamma(n+a+1) \Gamma(n+b+1)}{(2n+a+b+1) \Gamma(n+a+b+1) n!} \delta_{m,n},$$

where $\delta_{m,n}$ denotes the Kronecker delta. See [1, 7] for more details of orthogonal polynomials. Our method is applicable to almost general weight functions, however our method construct E-optimal designs approximately, not exactly, via approximate Tchebycheff functions. Next we define the approximate Tchebycheff functions, and its Tchebycheff points.

Definition 3.2. Suppose that the design space $\mathcal{X} = [-1, 1]$. For a general weight function $w(x)$ of regression such that if $-1 < x < 1$ then $w(x) > 0$, the function $\kappa^\dagger(x)$ obtained the following steps is called an approximate Tchebycheff function.

- (a) Compute the $(m - 1)$ -th degree of the orthogonal polynomial with respect to the weight function

$$\eta(x) = \frac{w(x)}{\sqrt{1 - x^2}}. \quad (8)$$

Let the orthogonal polynomial be $\nu_{m-1}(x)$, then

$$\nu_m(x) = \text{const.} \times \det \begin{pmatrix} c_0 & c_1 & c_2 & \dots & c_{m-1} \\ c_1 & c_2 & c_3 & \dots & c_m \\ \vdots & \vdots & \vdots & & \vdots \\ c_{m-2} & c_{m-1} & c_m & \dots & c_{2m-3} \\ 1 & x & x^2 & \dots & x^{m-1} \end{pmatrix}, \quad c_k = \int_{-1}^1 x^k d\eta(x).$$

The orthogonal polynomial $\nu_{m-1}(x)$ can be calculated by the above formula, or the Gram-Schmidt orthogonalization for example.

- (b) Obtain $\kappa^\dagger(x) = \mu_{m-1}(x)\sqrt{w(x)}$.

Then the Tchebycheff points $s_1^\dagger, s_2^\dagger, \dots, s_m^\dagger$ of the approximate Tchebycheff function $\kappa^\dagger(x)$ are defined as local maximum points and local minimum points.

Note that if the assumption $w(x) > 0$ for $-1 < x < 1$ is almost violated, approximate Tchebycheff functions and Tchebycheff points sometimes are not well-defined. However, in most cases, approximate Tchebycheff functions are similar to Tchebycheff functions. We show some examples of approximate Tchebycheff functions by Figures 1–2.

Figures 1–4 indicate that an approximate Tchebycheff function $\kappa^\dagger(x)$ has local maximums and local minimums whose absolute values are almost the same but not exactly the same. Figures 5–8 show the case where the assumption $w(x) > 0$ for $-1 < x < 1$ is almost violated, because $w(-1/2) = 0.001$ is close to 0. In this case the Tchebycheff points cannot be defined as local maximum points and local minimum points for $m = 4, 10, 20$.

It is also noted that if the weight function of regression is given by (6), then the approximate Tchebycheff function is equal to (7). Thus, in this case, the approximate Tchebycheff function is the exact Tchebycheff function.

By using the approximate Tchebycheff function, the proposed algorithm for calculating the approximation of E-optimal designs, as an approximate Tchebycheff designs, for weighted polynomial regression is described as follows.

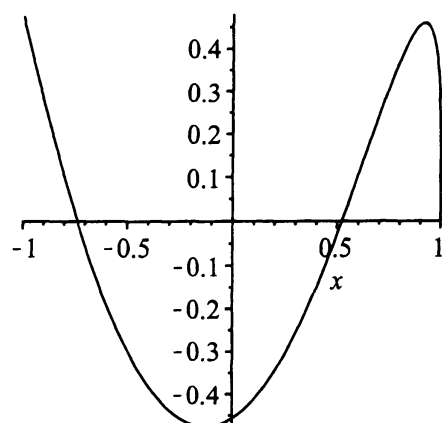


Figure 1: The approximate Tchebycheff function for $m = 3$, $w(x) = (1-x)^{1/2}(2+x)^{1/2}$

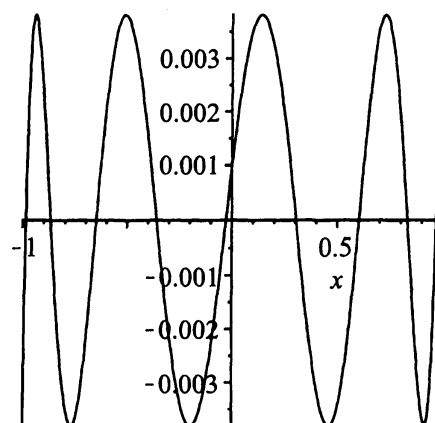


Figure 2: The approximate Tchebycheff function for $m = 10$, $w(x) = (1-x)^{1/2}(2+x)^{1/2}$

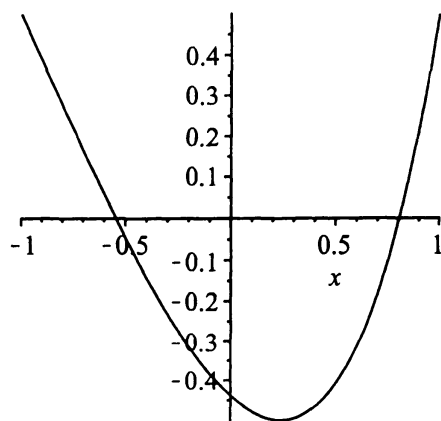


Figure 3: The approximate Tchebycheff function for $m = 3$, $w(x) = e^x$

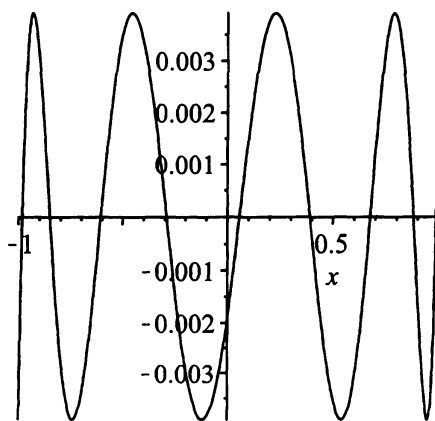


Figure 4: The approximate Tchebycheff function for $m = 10$, $w(x) = e^x$

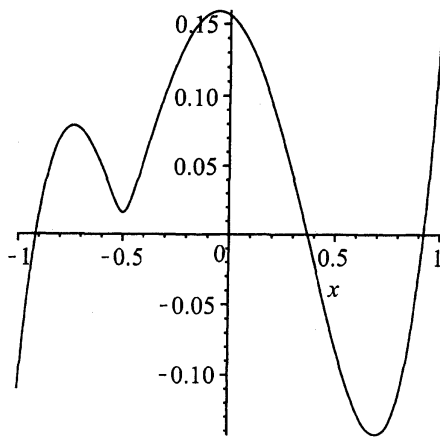


Figure 5: The approximate Tchebycheff function for $m = 4$, $w(x) = (x + 0.5)^2 + 0.001$

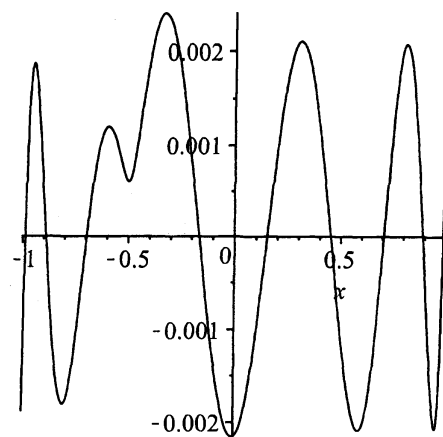


Figure 6: The approximate Tchebycheff function for $m = 10$, $w(x) = (x + 0.5)^2 + 0.001$

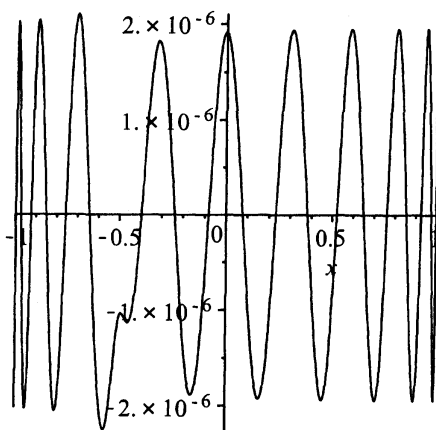


Figure 7: The approximate Tchebycheff function for $m = 20$, $w(x) = (x + 0.5)^2 + 0.001$

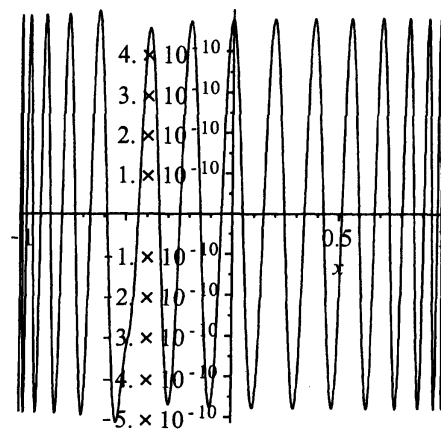


Figure 8: The approximate Tchebycheff function for $m = 32$, $w(x) = (x + 0.5)^2 + 0.001$

Algorithm 3.3. Suppose that the design space $\mathcal{X} = [-1, 1]$. For a general weight function $w(x)$ of regression such that if $-1 < x < 1$ then $w(x) > 0$, the design μ^\dagger is called the approximate Tchebycheff design.

- (a) Compute the approximate Tchebycheff function κ^\dagger by the Definition 3.2.
- (b) Compute the Tchebycheff points $s_1^\dagger, s_2^\dagger, \dots, s_m^\dagger$ of the approximate Tchebycheff function κ^\dagger .
- (c) Compute the design μ^\dagger given by

$$\mu^* = \begin{pmatrix} s_1^\dagger & s_2^\dagger & \cdots & s_m^\dagger \\ \rho_1 & \rho_2 & \cdots & \rho_m \end{pmatrix},$$

$$\begin{pmatrix} \rho_1 & \rho_2 & \cdots & \rho_m \end{pmatrix}^T = \frac{F^{-1}\gamma}{\gamma^T \gamma}, \quad F = \left((-1)^{j+1} f_{i-1}(s_j^\dagger) \right)_{i,j=1}^m.$$

In the next subsection, we show some results of numerical examples in order to verify that approximate Tchebycheff designs are close to E-optimal designs.

3.2 Numerical examples

In this subsection, we give numerical examples corresponding to the approximate Tchebycheff functions of Figures 1–4. These 4 examples indicate that approximate Tchebycheff designs have tendency to be close enough to E-optimal designs.

- (a) The case of $m = 3$, $w(x) = (1 - x)^{1/2}(2 + x)^{1/2}$: the corresponding Tchebycheff functions are shown in Figure 1. The approximate Tchebycheff design is

$$\mu^\dagger \approx \begin{pmatrix} -1.000 & -0.1252 & 0.9215 \\ 0.1721 & 0.4896 & 0.3383 \end{pmatrix}.$$

The optimal value of the optimization problem is

$$\lambda_{\min}(M_{f,w}(\mu^\dagger)) \approx 7.693 \times 10^{-3}.$$

The E-efficiency of the approximate Tchebycheff design $\text{eff}^E(\mu^\dagger)$ satisfies

$$1 - \text{eff}^E(\mu^\dagger) \approx 8.720^{-5},$$

where the E-efficiency is defined

$$\text{eff}^E(\mu^\dagger) = \frac{M_{f,w}(\mu^\dagger)}{\sup_{\mu} M_{f,w}(\mu)},$$

thus $1 - \text{eff}^E(\mu^\dagger)$ denotes a relative error in some sense. Here $\sup M_{f,w}(\mu)$ are calculated approximately by a random optimization.

- (b) The case of $m = 10$, $w(x) = (1 - x)^{1/2}(2 + x)^{1/2}$: the corresponding Tchebycheff functions are shown in Figure 2. The approximate Tchebycheff design is

$$\mu^\dagger \approx \begin{pmatrix} x_1 & x_2 & \cdots & x_{10} \\ \rho_1 & \rho_2 & \cdots & \rho_{10} \end{pmatrix},$$

where

$$\begin{aligned} x_1 &= -1.000, & \rho_1 &= 0.03909, \\ x_2 &= -0.9407, & \rho_2 &= 0.08305, \\ x_3 &= -0.7710, & \rho_3 &= 0.09785, \\ x_4 &= -0.5126, & \rho_4 &= 0.1201, \\ x_5 &= -0.1969, & \rho_5 &= 0.1395, \\ x_6 &= 0.1396, & \rho_6 &= 0.1423, \\ x_7 &= 0.4592, & \rho_7 &= 0.1261, \\ x_8 &= 0.7269, & \rho_8 &= 0.1031, \\ x_9 &= 0.9118, & \rho_9 &= 0.08509, \\ x_{10} &= 0.9949, & \rho_{10} &= 0.06379. \end{aligned}$$

The optimal value of the optimization problem is

$$\lambda_{\min}(M_{f,w}(\mu^\dagger)) \approx 1.714 \times 10^{-6}.$$

The E-efficiency of the approximate Tchebycheff design $\text{eff}^E(\mu^\dagger)$ satisfies

$$1 - \text{eff}^E(\mu^\dagger) \approx 3.334^{-5}.$$

- (c) The case of $m = 3$, $w(x) = e^x$: the corresponding Tchebycheff functions are shown in Figure 3. The approximate Tchebycheff design is

$$\mu^\dagger \approx \begin{pmatrix} -1.000 & 0.2405 & 1.000 \\ 0.3204 & 0.5360 & 0.1436 \end{pmatrix}.$$

The optimal value of the optimization problem is

$$\lambda_{\min}(M_{f,w}(\mu^\dagger)) \approx 1.976 \times 10^{-1}.$$

The E-efficiency of the approximate Tchebycheff design $\text{eff}^E(\mu^\dagger)$ satisfies

$$1 - \text{eff}^E(\mu^\dagger) \approx 4.082^{-8}.$$

- (d) The case of $m = 10$, $w(x) = e^x$: the corresponding Tchebycheff functions are shown in Figure 4. The approximate Tchebycheff design is

$$\mu^\dagger \approx \begin{pmatrix} x_1 & x_2 & \cdots & x_{10} \\ \rho_1 & \rho_2 & \cdots & \rho_{10} \end{pmatrix},$$

where

$$\begin{aligned} x_1 &= -1.000, & \rho_1 &= 0.04351, \\ x_2 &= -0.9326, & \rho_2 &= 0.09338, \\ x_3 &= -0.7416, & \rho_3 &= 0.1119, \\ x_4 &= -0.4566, & \rho_4 &= 0.1360, \\ x_5 &= -0.1190, & \rho_5 &= 0.1494, \\ x_6 &= 0.2267, & \rho_6 &= 0.1404, \\ x_7 &= 0.5399, & \rho_7 &= 0.1164, \\ x_8 &= 0.7876, & \rho_8 &= 0.09315, \\ x_9 &= 0.9457, & \rho_9 &= 0.07880, \\ x_{10} &= 1.000, & \rho_{10} &= 0.03710. \end{aligned}$$

The optimal value of the optimization problem is

$$\lambda_{\min}(M_{f,w}(\mu^\dagger)) \approx 1.660 \times 10^{-6}.$$

The E-efficiency of the approximate Tchebycheff design $\text{eff}^E(\mu^\dagger)$ satisfies

$$1 - \text{eff}^E(\mu^\dagger) \approx 2.998^{-9}.$$

3.3 Properties and conjectures

In previous subsection, we ascertain that approximate Tchebycheff designs have tendency to be close to E-optimal designs. Here we show that exact Tchebycheff designs gives E-optimal designs for weighted polynomial regression if regression has a unique E-optimal design.

Theorem 3.4. *Let $w(x)$ be the weight function of polynomial regression with the design space \mathcal{X} , and let $g_k(x) = x^k \sqrt{w(x)}$. Then the set $\{g_0(x), g_1(x), \dots, g_{m-1}(x)\}$ is a weak Tchebycheff system on \mathcal{X} . Let polynomial regression with weight function $w(x)$ have a unique E-optimal design. Then the Tchebycheff system is the E-optimal design.*

Proof. This theorem can be shown by using [4, pp. 9–20] and [4, Theorem II 10.2]. \square

We have the following conjecture, which is derived from Figures 5–8 for examples.

Conjecture 3.5. *Approximate Tchebycheff functions converge exact Tchebycheff functions in some sense as m goes to infinity.*

At last, we note that if the design space is $\mathcal{X} = [a, b]$, then we can discuss the almost same results by using

$$\eta(x) = \frac{w(x)}{\sqrt{(x-a)(b-x)}}$$

instead of (8).

4 Conclusions

In this paper, we first indicate a new definition of approximate Tchebycheff functions. By using this definition, we propose a new algorithm for constructing the approximate Tchebycheff designs for weighted polynomial regression with almost general weight functions. After that, we verify that the approximate Tchebycheff designs are close to E-optimal designs by numerical examples.

As future works, it is necessary to discuss the definition of approximate Tchebycheff functions more strictly. We must clarify how much gaps of the absolute values of local maximums and local minimums of approximate Tchebycheff functions are admitted.

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